

SENSITIVITY EQUATION DERIVATION FOR TRANSIENT HEAT TRANSFER PROBLEMS

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ABSTRACT

The focus of the paper is on the derivation of sensitivity equations for transient heat transfer problems modeled by different discretization processes. Two examples will be used in this study to facilitate the discussion. The first example is a coupled, transient heat transfer problem that simulates the press molding process in fabrication of composite laminates. These state equations are discretized into standard h -version finite elements and solved by a multiple step, predictor-corrector scheme. The sensitivity analysis results based upon the direct and adjoint variable approaches will be presented. The second example is a nonlinear transient heat transfer problem solved by a p -version time-discontinuous Galerkin's Method. The resulting matrix equation of the state equation is simply in the form of $Ax = b$, representing a single step, time marching scheme. A direct differentiation approach will be used to compute the thermal sensitivities of a sample 2D problem.

INTRODUCTION

Sensitivity analysis is defined in this paper as a process that derives sensitivity equations to compute the derivatives of responses or states with respect to specified variables. Since the derivative information can greatly enhance the robustness and accuracy of curve fitting, sensitivity analysis becomes a necessary element in many engineering applications. Examples include design trade-off, weather prediction, analysis error correction, model adjustment, reliability analysis and design optimization.

In sensitivity analysis, the response or dependent variable can be a real number, a function or a functional and the independent variable can be a real number or a function. The challenge of sensitivity analysis arises when the responses to be differentiated involve the solutions of some governing equations. In these cases, the

responses or states are implicitly related to the independent variables through the governing equations. These governing state equations can be expressed as differential, integral or algebraic forms. The latter is usually as a result of numerical discretization of the former.

Many approaches are available for sensitivity analysis, including automatic differentiation¹, complex variable method², finite differencing, or more traditional analytical approaches³⁻⁶. The analytical approaches used for sensitivity analysis can be further classified into various categories. It can be classified as the discrete approach or the distributed (continuous) approach, based upon which types of governing equations, responses and independent variables are considered. The discrete approach works with discretized algebraic equations and real numbers, while the distributed approach works with functionals and functions. Sensitivity analysis can also be classified as the direct differentiation approach or the adjoint variable approach, based upon whether the derivatives of the state variables are computed explicitly in the process. The bulk of the effort of the direct differentiation method is to establish a sensitivity equation solved for the derivatives of state variables, whereas the effort of the adjoint approach is to form and solve an adjoint equation and eventually, compute the derivatives of the responses without explicitly computing the derivatives of the state variables.

Subjects related to sensitivity analysis of dynamic transient problems can be found in the literature^{3-4,6}. Thermal transient analysis can be performed in the similar fashion⁷⁻⁹. Recent development and applications of thermal transient analysis can be found in aerospace applications¹⁰⁻¹¹, laser surface treatment¹², material processes¹³⁻¹⁴, and their references. The major focus of the report is on the derivation of sensitivity equations for transient heat transfer problems represented in various forms of governing equations. Two examples will be used in this study to facilitate the discussion.

The first example is a coupled, transient heat transfer problem that simulates the press molding process in fabrication of composite laminates. The state equations are made of a heat conduction equation that calculates the through-thickness temperature distribution and an empirical equation that monitors the chemical-kinetic reaction of resins. These state equations are discretized into standard h -version finite elements and expressed in the form of $A\dot{\mathbf{x}} + B\mathbf{x} = \mathbf{c}$. The resultant equations are then solved by a multiple step, predictor-corrector scheme. Both of the direct and adjoint variable approaches will be used to derive the sensitivity equations in continuous forms. The numerical implementation aspects of those sensitivity equations and their accuracies will be studied in this paper.

The second example is a nonlinear transient heat transfer problem solved by a p -version, time-discontinuous Galerkin's Method¹⁵⁻¹⁷. The resulting matrix equation of the state equation is simply in the form of $A\mathbf{x} = \mathbf{b}$, representing a single step, time marching scheme. A direct differentiation approach is used to compute the thermal

sensitivities of a simple 2 D heat conduction problem. Here, possible usages of the sensitivity results are presented.

EXAMPLE 1: *h*-VERSION FINITE ELEMENT APPROXIMATION

The interest of this study is in compression molding of a filled polyester resin reinforced by chopped glass fibers. The unmolded composite is produced in sheets which are from 3 to 6 mm thick, typically. The resin consists of a thick dough and the chopped fibers (about 25 mm long) which are randomly oriented in the plane of the sheet. In this form, the material is called sheet molding compound, or simply SMC¹⁸. A diffusion reaction system in terms of the temperature distribution and the degree of cure can be used to describe the cure process of the composite material under consideration.

The system equations can be expressed as

$$\rho c \frac{\partial u}{\partial t} - k \frac{\partial^2 u}{\partial x^2} = \rho H_r \frac{\partial \alpha}{\partial t}, \quad \text{in } (0, h) \times (0, \tau] \quad (1)$$

$$u(h, t) = u_c(t) \quad \text{on } (0, \tau] \quad (2)$$

$$\frac{\partial u(0, t)}{\partial x} = 0 \quad \text{on } (0, \tau] \quad (3)$$

and

$$u = u_0(x), \quad \text{in } (0, h) \text{ at } t=0 \quad (4)$$

where ρ and c are the density and the specific heat of the composite material, respectively, k is the thermal conductivity in the direction perpendicular to the plane of composite material, $2h$ is the total thickness, $u_c(t)$ is the cure cycle in K° , τ is the time in seconds needed for the completion of one cure cycle, H_r is the total or ultimate heat of reaction, and the last term in Eq. 1, $\rho H_r \frac{\partial \alpha}{\partial t}$, is the rate of heat generated by the chemical reaction as characterized by the degree of cure α .

The degree of cure, α , is defined as the fraction of heat, $H(t)$, released up to time, t , for the resin system under cure; $\alpha = H(t) / H_r$. Both $H(t)$ and H_r in Eq. 4 can be measured experimentally by Differential Scanning Calorimetry (DSC). For an uncured material, α approaches zero, and for a completely cured material, α approaches one. The reaction rate, $\frac{\partial \alpha}{\partial t}$, depends strongly on the curing temperature. As an example, the cure rate equation of a stepwise isothermal curing process which can be used for a polyester SMC is described as follows:

$$\begin{aligned}
\frac{\partial \alpha}{\partial t} &= f(\alpha, T) \\
&= (K_1 + K_2 \alpha^m)(1 - \alpha)^n \\
&= (a_1 e^{-d_1/RT} + a_2 e^{-d_2/RT} \alpha^m)(1 - \alpha)^n
\end{aligned} \tag{5}$$

where a_1, a_2, d_1, d_2, m and n are constants, R is the universal gas constant, and K_1 and K_2 are exponential functions of the temperature.

The optimal cure cycle design¹⁹ aims to select the profile of cure temperature, $u_c(t)$, to achieve the following goals in a compress molding process.

- a) The maximum temperature inside the composite during the cure process can not be too high to avoid buring.
- b) The material is cured completely at the end of the cure process.
- c) The material is cured uniformly at any time during the cure process.

The first two objectives may be mathematically formulated as point-wise functions,

$$\begin{aligned}
T(t) &\leq T_f & \text{in} & \quad [0, h] \times [0, \tau] \\
\alpha(x, \tau) &\geq \alpha_f & \text{in} & \quad [0, h]
\end{aligned}$$

where τ is the total time required to complete one cure cycle. Furthermore, the last objective may be measured by the temperature uniformity, which is expected to lead to the uniformity of the curing reaction. Mathematically, the temperature uniformity is represented by the least-square integral of the deviation between the point-wise temperature and the averaged temperature as

$$\psi_0 = \int_0^\tau \int_0^h u^2 dx - \left(\int_0^h u dx \right)^2 / h \tag{6}$$

To support the optimal cure cycle design, the thermal design derivatives of the functional, ψ_0 , the temperature, $u(x, t)$ and the degree of cure, $\alpha(x, t)$, with respect to the cure temperature, $u_c(t)$, are required.

Note that the cure temperature appears as a part of the non-homogeneous boundary equation in Eq. 2. By using the following replacement of the temperature, $u(x, t)$, by $\bar{u}(x, t)$ as

$$u(x, t) = \bar{u}(x, t) + u_c(t) \tag{7}$$

which leads to simplification of the heat conduction equation, Eq. 1,

$$\rho c \frac{\partial \bar{u}}{\partial t} = k \frac{\partial^2 \bar{u}}{\partial x^2} - \rho c \frac{\partial u_c}{\partial t} + \rho H_r f(\alpha, \bar{u} + u_c)$$

with the homogeneous boundary equations

$$\bar{u}(h,t) = 0, \quad \text{in } [0, \tau] \quad (8)$$

$$\frac{\partial \bar{u}(0,t)}{\partial x} = 0, \quad \text{in } [0, \tau] \quad (9)$$

and the initial condition,

$$\bar{u}(x,0) = u_0(x) - u_c(0), \quad \text{in } [0,h] \quad (10)$$

where f is defined in Eq. 5. Since the initial temperature, $u_0(t)$ is the same as the initial cure temperature for most applications, Eq. 10 may yield a homogeneous initial condition as well. From here on, $\bar{u}(x,t)$ is abbreviated as $u(x,t)$ for simplification.

The weak forms of the above equation can now be derived based upon the Galerkin's method for arbitrary functions, $w(x)$ and $s(x)$, as

$$\pi_u = 0 = \int_0^h \left(\rho c \frac{\partial u}{\partial t} - k \frac{\partial^2 u}{\partial x^2} + \rho c \frac{du_c}{dt} - \rho H_r f \right) w dz \quad (11)$$

and

$$\pi_\alpha = 0 = \int_0^h \left(\frac{\partial \alpha}{\partial t} - f \right) s dx \quad (12)$$

THERMAL SENSITIVITY ANALYSIS

The system equation of Eqs. 1-5 simply reveals the fact that their solutions, $u(x,t)$ and $\alpha(x,t)$ are functions of the design variable, $u_c(t)$. However, since the design variable $u_c(t)$ itself is a function, the thermal derivative of $u(x,t)$ with respect to $u_c(t)$ can be defined as the variation of $u(x,t)$, δu , due to the variation in $u_c(t)$, δu_c ,

$$\delta u = \frac{d}{d\varepsilon} u(x,t; u_c + \varepsilon \delta u_c) \Big|_{\varepsilon=0}$$

The cure derivative, $\delta \alpha$ can be defined similarly.

The variation of the functional defined in Eq. 6 is then given as

$$\delta \psi = \int_0^\tau \left[\int_0^h 2u - \frac{2}{h} \int_0^h u dx \right] \delta u dx dt \quad (13)$$

It is assumed that $u(x, t; u_c)$ and $\alpha(x, t; u_c)$ have enough regularity in the time-spatial domain and in the design space. Thus, the order of the differentiation and the variation is exchangeable; therefore,

$$\begin{aligned}\frac{\partial(\delta u)}{\partial t} &= \delta\left(\frac{\partial u}{\partial t}\right) \\ \frac{\partial(\delta \alpha)}{\partial t} &= \delta\left(\frac{\partial \alpha}{\partial t}\right)\end{aligned}$$

and

$$\frac{\partial^2(\delta u)}{\partial x^2} = \delta\left(\frac{\partial^2 u}{\partial x^2}\right)$$

With the aid of the above equations, the variations of the state equations defined by Eq. 11 - 12 yield

$$\begin{aligned}0 = \int_0^\tau \int_0^h \left(\rho c \frac{\partial \delta u}{\partial t} \lambda + \rho c \frac{d(\delta u_c)}{dt} \lambda - \rho \frac{\partial^2(\delta u)}{\partial x^2} \lambda - \rho H_r \frac{\partial f}{\partial \alpha} \delta \alpha \lambda \right. \\ \left. - \rho H_r \frac{\partial f}{\partial u} \delta u \lambda - \rho H_r \frac{\partial f}{\partial u_c} \delta u_c \lambda \right) dx dt, \quad (14)\end{aligned}$$

and

$$0 = \int_0^\tau \int_0^h \left(s \delta \frac{\partial(\delta \alpha)}{\partial t} - s \frac{\partial f}{\partial \alpha} \delta \alpha - s \frac{\partial f}{\partial u} \delta u - s \frac{\partial f}{\partial u_c} \delta u_c \right) dx dt. \quad (15)$$

Integrating by parts simplify the above equation as

$$\begin{aligned}0 = \int_0^\tau \int_0^h \left[\left(-\rho c \frac{\partial \lambda}{\partial t} - k \frac{\partial^2 \lambda}{\partial x^2} - \rho H_r \lambda \frac{\partial f}{\partial u} \right) \delta u + \left(-\rho c \frac{\partial \lambda}{\partial t} - \rho H_r \lambda \frac{\partial f}{\partial u_c} \right) \delta u_c \right. \\ \left. - \rho H_r \lambda \frac{\partial f}{\partial \alpha} \delta \alpha \right] dx dt + \int_0^\tau k \frac{\partial \lambda}{\partial x} \delta u \Big|_0^h dt \\ - \int_0^\tau k \lambda \frac{\partial(\delta u)}{\partial x} \Big|_0^h dt + \int_0^h \rho c \lambda \delta u \Big|_0^\tau dx + \int_0^h \rho c \lambda \delta u_c \Big|_0^\tau dx, \quad (16)\end{aligned}$$

and

$$\begin{aligned}
0 = & \int_0^\tau \int_0^h \left(-\frac{\partial s}{\partial t} \delta \alpha - s \frac{\partial f}{\partial \alpha} \delta \alpha - s \frac{\partial f}{\partial u} \delta u - s \frac{\partial f}{\partial u_c} \delta u_c \right) dx dt \\
& + \int_0^h s \delta \alpha \Big|_0^\tau dx.
\end{aligned} \tag{17}$$

THE ADJOINT VARIABLE APPROACH

Adding Eqs. 13, 16, and 17 up, one has the variation of the functional ψ as

$$\begin{aligned}
\delta \psi = & \int_0^\tau \int_0^h \left[\left(2u - \frac{2}{h} \int_0^h u dz \right) - \rho c \frac{\partial \lambda}{\partial t} - k \frac{\partial^2 \lambda}{\partial x^2} - \rho H_r \frac{\partial f}{\partial u} - s \frac{\partial f}{\partial u} \right] \delta u dx dt \\
& + \int_0^\tau \int_0^h \left(-\rho H_r \lambda \frac{\partial f}{\partial \alpha} - \frac{\partial s}{\partial t} - s \frac{\partial f}{\partial \alpha} \right) \delta \alpha dx dt \\
& + \int_0^\tau \int_0^h \left(-\rho c \frac{\partial \lambda}{\partial t} - \rho H_r \lambda \frac{\partial f}{\partial u_c} - s \frac{\partial f}{\partial u_c} \right) \delta u_c dx dt \\
& + \int_0^h \rho c \lambda \delta u_c \Big|_0^\tau + \int_0^\tau k \frac{\partial \lambda}{\partial x} \delta u \Big|_0^h dt - \int_0^\tau k \lambda \frac{\partial \delta u}{\partial x} \Big|_0^h dt \\
& + \int_0^h \rho c \lambda \delta u_c \Big|_0^\tau dx + \int_0^h s \delta \alpha \Big|_0^\tau dx
\end{aligned} \tag{18}$$

Note that $\lambda(x, t)$ and $s(x, t)$ are arbitrary functions, and the design derivatives δu and $\delta \alpha$ are the only two unknowns in the above equation. One may now specify the variables λ and s in such a way that all of the terms associated with δu and $\delta \alpha$ are dropped. This can be accomplished by introducing the following adjoint equations for λ and s as:

$$0 = \rho c \frac{\partial \lambda}{\partial t} + k \frac{\partial^2 \lambda}{\partial x^2} + \rho H_r \frac{\partial f}{\partial u} + s \frac{\partial f}{\partial u} - \left(2u - \frac{2}{h} \int_0^h u dx \right) \tag{19}$$

and

$$0 = \frac{\partial s}{\partial t} + \rho H_r \lambda \frac{\partial f}{\partial \alpha} + s \frac{\partial f}{\partial \alpha} \tag{20}$$

with the terminal conditions,

$$\lambda(0, \tau) = 0, \quad \text{in } [0, h] \tag{21}$$

$$s(x, \tau) = 0, \quad \text{in} \quad [0, h] \quad (22)$$

and the boundary conditions,

$$\frac{\partial \lambda}{\partial x}(0, t) = 0, \quad \text{in} \quad [0, \tau] \quad (23)$$

$$\lambda(h, t) = 0, \quad \text{in} \quad [0, \tau] \quad (24)$$

Thus, the combination of Eqs. 18 - 24 provides a simple formula for the design derivative of the functional,

$$\begin{aligned} \delta\psi = & \int_0^\tau \int_0^h \left(-\rho c \frac{\partial \lambda}{\partial t} - \rho H_r \frac{\partial f}{\partial u_c} - s \frac{\partial f}{\partial u_c} \right) \delta u_c dx dt \\ & + \int_0^h \rho c \lambda(0) \delta u_c(0) dx \end{aligned} \quad (25)$$

Equation 25 shows that the design derivative of ψ , namely, $\delta\psi$, is a functional of state variables α and u , and the adjoint variables λ and s . The matrix equations which solve the nodal values of α and u can be formed by the standard h -version finite element method as.

$$C \dot{\alpha} + K \alpha = q \quad (26)$$

$$M \dot{\alpha} = r \quad (27)$$

Since the adjoint variables of Eqs. 19 – 20 form an “adjoint” diffusion-reaction system similar to the original one, the same numerical scheme used to solved the state variables α and u can be extended here to compute the adjoint variables λ and s . For instance, using the same shape functions of u and α to interpolate the adjoint variables λ and s obtains the following matrix equation for nodal value of λ and s in the form of

$$C \dot{\lambda} - K \lambda = q^* \quad (28)$$

and

$$M \dot{s} = r^* \quad (29)$$

with proper boundary and terminal conditions.

In general, the adjoint equation cannot be solved simultaneously alongside with the original system equation. Because of the terminal conditions, the adjoint equations can be solved by either the backward integration along the real time t – axis directly or the forward integration along the artificial time t^* - axis, provided that the

independent variable t is changed to t^* as $t^* = \tau - t$. However, both approaches require the solution of the original system equation known prior to solving the adjoint equations.

THE DIRECT DIFFERENTIATION METHOD

The direct differentiation method is an approach that differentiates the governing equations with respect to a design variable directly. The variation δu in $\delta \psi$ of Eq. 13 and $\delta \alpha$ can be obtained by solving the equations, $\delta \pi_\alpha = 0$ and $\delta \pi_u = 0$, in their weak forms such as Eqs. 14-15, or in their differential forms as

$$\begin{aligned} \rho c \frac{\partial(\delta u)}{\partial t} &= k \frac{\partial^2(\delta u)}{\partial x^2} - \rho c \frac{\partial(\delta u c)}{\partial t} + \rho H_r \frac{\partial f}{\partial \alpha} \delta \alpha \\ &+ \rho H_r \frac{\partial f}{\partial u} \delta u + \rho H_r \frac{\partial f}{\partial u_c} \delta u_c \end{aligned} \quad (30)$$

and

$$\frac{\partial(\delta \alpha)}{\partial t} = \frac{\partial f}{\partial \alpha} \delta \alpha + \frac{\partial f}{\partial u} \delta u + \frac{\partial f}{\partial u_c} \delta u_c \quad (31)$$

where the design variable variation, δu_c , is known.

Again, Eqs. 14-15 or Eqs. 30-31 can be discretized into finite element matrix equations, similar to Eqs. 26-27 as δu and $\delta \alpha$ can be interpolated by the same shape functions as u and α . These equations can be symbolically written as

$$C \dot{\mathbf{a}}_b + K \mathbf{a}_b = \mathbf{q}_b \quad (32)$$

$$M \dot{\boldsymbol{\alpha}}_b = \mathbf{r}_b \quad (33)$$

where δu and $\delta \alpha$ are interpolated by the same shape functions as u and α , in which \mathbf{a}_b and $\boldsymbol{\alpha}_b$ are the nodal vectors of δu and $\delta \alpha$.

NUMERICAL RESULTS

The initial-value problems of the state variables, their thermal derivatives and corresponding adjoint variables are all solved by the computer code, DE²⁰. The DE program is one of predictor-corrector integration algorithms using Adams family of

formulas. The truncation error is controlled by varying both the step size and the order of the polynomial approximation. The DE program is quite easy to use and has the capability to manage moderate stiff equations which happen commonly in the problems of chemical kinetics. To maintain a unified accuracy in the analysis, the computation of two state variables, namely, the temperature and the degree of cure, are subjected to the same error tolerance in this study.

Note that the coefficient matrices of \mathbf{a}_b and $\boldsymbol{\alpha}_b$ in Eqs. 32-33 are identical to those of \mathbf{a} and $\boldsymbol{\alpha}$ defined in Eqs. 26-27. Therefore, the same numerical scheme and the numerical tolerance can be applied to solve both Eq. 26-27, and 32-33 simultaneously for state variables, \mathbf{a} and $\boldsymbol{\alpha}$, and design derivatives, \mathbf{a}_b and $\boldsymbol{\alpha}_b$. In this way, the state variables and the design derivatives can enjoy the same numerical accuracy.

Regarding the computational efficiency, it is worthwhile mentioning two notes here:

- a) Because the coefficient matrices of Eqs. 32-33 are identical to those of Eqs. 26-27, the triangular factorizations of matrices \mathbf{C} and \mathbf{M} are needed to be done only once.
- b) Compared to the original system equations, the right hand sides of the equations for computing \mathbf{a}_b and $\boldsymbol{\alpha}_b$, such as Eqs. 32-33, may have different frequency contents. Thus, to maintain the same numerical accuracy, a small time step Δt may be required for the DE program to solve the pairs $(\mathbf{a}, \boldsymbol{\alpha})$ and $(\mathbf{a}_b, \boldsymbol{\alpha}_b)$, simultaneously.

Once \mathbf{a} and \mathbf{a}_b are available, the design derivative given in Eq. 13 can be easily obtained by numerical integration. Another suggestion is to rewrite the integral form of Eq. 13 as a differential equation of $\delta\psi$ given as

$$\frac{d\delta\psi}{dt} = \int_0^h \left[2u - \frac{2}{h} \int_0^h u dz \right] \delta u dz \quad (34)$$

The above ordinary differential equation of $\delta\psi_b$ can then be solved simultaneously with equations of $(\mathbf{a}, \boldsymbol{\alpha})$ and $(\mathbf{a}_b, \boldsymbol{\alpha}_b)$. In this way, one extra equation of design derivative $\delta\psi$ for each design variable is added in the design sensitivity analysis. However, the accuracy of $\delta\psi$ is secured. Eq. 34 is used to generate the current numerical results.

An example which deals with the cure process of compression molding is presented in this section to discuss the numerical accuracy of the adjoint variable method and the direct differentiation method for calculating the thermal design derivatives. The accuracy of the thermal design sensitivity can be checked by using the fundamental definition of design derivatives which can be approximated by the finite difference.

The finite perturbation of the design variable, Δb , is defined as the difference between a perturbed design b^* and the nominal design b , i.e., $\Delta b = b^* - b$. As a result, it follows that

$$\begin{aligned}\Delta\psi &= \psi(b^*) - \psi(b) \\ &\equiv \psi' \Delta b\end{aligned}\tag{35}$$

The above equation provides a simple means to check the accuracy of the design sensitivity analysis. Nevertheless, the difficulty of this method is the selection of Δb . If Δb is too large, the approximation in Eq. 35 is not valid. On the other hand, if Δb is too small, the round-off error in the computation of $[\psi(b^*) - \psi(b)]$ becomes too large to ensure the validity of Eq. 35.

The first example present here deals with the cure process in which the cure temperature of the process is assumed to be a constant temperature. The nominal cure temperature is taken as 423° k. According to the approximation defined in Eq. 35, the results of $\Delta\psi$ and Δb shown in Fig. 1 demonstrate that the thermal design sensitivity calculated by the direct differentiation method is more accuracy than the results calculated by adjoint variable method. Moreover, by using the direct differentiation method, one can also get the time histories of the design derivatives of state variables as shown in Figs. 2 and 3.

EXAMPLE 2: *p*-VERSION, TIME-DISCONTINUOUS FINITE ELEMENT APPROXIMATION

This example will examine a more general heat conduction equation than the one presented in Eq. 1. The governing differential equation is given as

$$\rho c \frac{\partial u}{\partial t} - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \left[k_{ij} \frac{\partial u}{\partial x_j} \right] = Q(x, t), \quad \text{in } \Omega \times (0, T] \tag{36}$$

$$u = f(x, t) \quad \text{on } \partial\Omega_u \times (0, T] \tag{37}$$

$$\sum_{i=1}^3 \sum_{j=1}^3 k_{ij} \frac{\partial u}{\partial x_j} [n_i] = q_s(x, t), \quad \text{on } \partial\Omega_q \times (0, T] \tag{38}$$

$$\sum_{i=1}^3 \sum_{j=1}^3 k_{ij} \frac{\partial u}{\partial x_j} [n_i] = -h(u - T_\infty), \quad \text{on } \partial\Omega_h \times (0, T] \tag{39}$$

and

$$u = g(x), \quad \text{in } \Omega \text{ at } t = 0 \tag{40}$$

where the temperature, $u(x, t)$, is the only unknown. Eq. 36 represents an initial-boundary value problem with Eqs. 37-39 being the temperature, the heat flux

boundary condition, and the thermal convective condition; respectively, and Eq. 40, the initial conditions. It is assumed that the heat source, Q , the prescribed temperature, f , the flux, q_s , the thermal film coefficient, h , and the initial value, g , are all with proper regularity. In case of material nonlinearity, the specific heat, $\rho c(u)$, the film coefficient, $h(u)$, and the thermal conductivity, $k_{ij}(u)$ are assumed to be functions of temperature.

Let $f = 0$ on Ω_u . Otherwise, u in Eqs.36-40 can be replaced by $u - f$ to achieve a homogenous boundary condition on Ω_u . As a result, the weak form of Eqs. 36-40 can be derived, based upon the Galerkin's Method for an arbitrary function, $w(\mathbf{x})$, as

$$\begin{aligned} & \int_{\Omega} \left(\rho c \frac{\partial u}{\partial t} w + \sum_{i=1}^3 \sum_{j=1}^3 k_{ij} \frac{\partial u}{\partial x_i} \frac{\partial w}{\partial x_j} \right) dv + \int_{\partial\Omega_h} h u w ds \\ &= \int_{\Omega} Q w dv + \int_{\partial\Omega_q} q_s w ds + \int_{\partial\Omega_h} h T_{\infty} w ds \end{aligned} \quad (41)$$

In the approach of time-discontinuous Galerkin's method that is under development in this study, the time coordinate is treated as the same as the spatial coordinate. The time space is also discretized into elements or intervals. Focusing on one time interval, $I_n = [t_{n-1}, t_n)$, the weak form, Eq. 41, can be extended to the entire product domain $I_n \times \Omega$

$$\begin{aligned} & \int_{n-1}^n \left[\int_{\Omega} \left(\rho c \frac{\partial u}{\partial t} w + \sum_{i=1}^3 \sum_{j=1}^3 k_{ij} \frac{\partial u}{\partial x_i} \frac{\partial w}{\partial x_j} \right) dv \right] dt + \int_{n-1}^n \left[\int_{\partial\Omega_h} h u w ds \right] dt \\ &= \int_{n-1}^n \left[\int_{\Omega} Q w dv + \int_{\partial\Omega_q} q_s w ds + \int_{\partial\Omega_h} h T_{\infty} w ds \right] dt \end{aligned} \quad (42)$$

where, $w(\mathbf{x}, t)$ is the testing function. Furthermore, to enforce the continuous requirement at the interfaces of time intervals, a weighted integral form of constraint, is appended to Eq. 42

$$\int_{\Omega} (\rho c^+ u^+ - \rho c^- u^-) w^+ dv = 0 \quad (43)$$

In this example, the temperature, $u(\mathbf{x}, t)$, is interpolated by a p -version hierarchical basis functions as

$$\begin{aligned} u(\mathbf{x}, t) &= \chi^T(\mathbf{x}, y, z, t) \mathbf{a} \\ &= (\phi(\mathbf{x}, y) \otimes \psi(z) \otimes \theta(t))^T \mathbf{a} \end{aligned} \quad (44)$$

The symbol, \otimes , represents the outer tensor product operator and the vectors, ϕ , ψ and θ , represent collections of basis functions. Particularly, the through-thickness basis functions, ψ , are made of the Legendre polynomials of the first kind¹⁵, the temporal basis functions, θ , the integrations of the same Legendre polynomials and the in-plane basis functions, ϕ , chosen for triangular elements, as described by reference 21.

It is assumed that in this study, the film coefficient h is set to zero and the relations between the other material properties, ρc and K_{ij} , and the temperature are defined in a tabulated form, presented as a result of experiments. Therefore, the material properties cannot be explicitly specified as functions of position and time as required by integration. An approximation is thus introduced to overcome such a difficulty. The standard Lagrange polynomials are used here for this purpose.

The values of the material properties at the Lagrange points are taken from a given material table based upon the values of the temperature found at those points. The values of the material properties at elsewhere in an element are then obtained through interpolation. In this way, the material properties can be explicitly approximated as functions of position and time throughout the problem domain.

As an example, the material property, say ρc , can be interpolated in an element ($I_n \times \Omega_p$) as

$$\begin{aligned}\rho c(\mathbf{x}, t) &= (N_c(x, y, z, t))^T \boldsymbol{\delta}_c \\ &= (N_{cp}(x, y) \otimes N_{cz}(z) \otimes N_{ct}(t))^T \boldsymbol{\delta}_c \\ &= \sum_i \sum_j \sum_k (N_{cpi}(x_i, y_i) \otimes N_{czj}(z_j) \otimes N_{ctk}(t_k))^T \delta_{cijk}\end{aligned}\quad (45)$$

where, δ_{cijk} is a component of the vector, $\boldsymbol{\delta}_c$, which takes the value of the material properties found in the material table.

If the material properties are interpolated linearly through the tabulated data, the value of the materials can be represented as, using ρc as an example,

$$\delta_{cijk} = \alpha_{ijk} + \beta_{ijk} u_{ijk}$$

where α_{ijk} and β_{ijk} are constants taken from the material table based upon the temperature value, u_{ijk} , measured at the location (x_i, y_i, z_j) and at time t_k as

$$\begin{aligned}u_{ijk} &= \chi_{ijk}^T \mathbf{a} \\ &= (\phi(x_i, y_i) \otimes \psi(z_j) \otimes \theta(t_k))^T \mathbf{a}\end{aligned}$$

SYSTEM EQUATION

Once the interpolation functions are selected and the nonlinear material properties are approximated as explicit functions of position and time, one can proceed to integrate the terms in Eqs.42-43 to construct the equivalent matrices. The resultant finite element matrix equation for the time interval, I_n , can then be expressed as

$$[C_n(\mathbf{a}_n) + K_n(\mathbf{a}_n) + M_n^+(\mathbf{a}_n)]\mathbf{a}_n = \mathbf{q}_n + [M_{n-1}^-(\mathbf{a}_{n-1})]\mathbf{a}_{n-1} + \mathbf{b}_n \quad (46)$$

where the subscript, n , indicates that the associated matrix or vector is evaluated with functions defined in time interval, I_n . Note that each term in Eq.46 is corresponding to an integral in Eqs. 42-43, which can be evaluated based upon the interpolation functions of Eqs. 44-45. As an example, the capacitance matrix is given as

$$\begin{aligned} C_n &= \sum_p C_{\Omega_p} \\ &= \sum_p \int_{t_{n-1}}^{t_n} \left(\int_{\Omega_n} \rho c \frac{\partial u}{\partial t} w dx \right) dt \end{aligned}$$

The details of an elemental capacitance matrix, C_{Ω_p} is given as Eq. A.1 in Appendix.

The matrix equation derived above is based upon the discontinuous Galerkin's method and will be solved in a time-marching fashion. In other words, the matrix equation of Eq. 46 will be solved for a time interval at a time, with \mathbf{a}_n as unknown and \mathbf{a}_{n-1} as known quantities. Because its nonlinear nature, Eq. 46 can be solved by the Newton-Raphson's method, which leads to a recursive formula

$$[C_n(\mathbf{a}_n^{i-1}) + K_n(\mathbf{a}_n^{i-1}) + M_n^+(\mathbf{a}_n^{i-1}) + J_c(\mathbf{a}_n^{i-1}) + J_k(\mathbf{a}_n^{i-1}) + J_m(\mathbf{a}_n^{i-1})]\Delta\mathbf{a}_n^i = -\mathbf{R}_n^{i-1} \quad (47)$$

and the solution is updated by

$$\mathbf{a}_n^i = \mathbf{a}_n^{i-1} + \Delta\mathbf{a}_n^i \quad (48)$$

In the above equation, $\Delta\mathbf{a}_n^i$ is the improvement of the solution and \mathbf{R}_n^{i-1} is the residual of the nonlinear equation at the $i-1$ iteration, which is defined as

$$\mathbf{R}_n^{i-1} = [C_n(\mathbf{a}_n^{i-1}) + K_n(\mathbf{a}_n^{i-1}) + M_n^+(\mathbf{a}_n^{i-1})]\mathbf{a}_n^{i-1} - \mathbf{q}_n - [M_{n-1}^-(\mathbf{a}_{n-1})]\mathbf{a}_{n-1} - \mathbf{b}_n$$

Moreover, the derivative matrices, J_c , J_k and J_m are obtained by differentiating the coefficient matrices C_n , K_n and M_n^+ with respect to the unknown vector \mathbf{a}_n , respectively. This is usually accomplished at the element level. As an example, the derivative matrix, J_c , is detailed in Appendix as Eq. A.2.

SENSITIVITY ANALYSIS

Since the matrix equation, Eq. 46 , is in the form of a static problem, $A\mathbf{x}=\mathbf{b}$. Differentiation of Eq. 46 with respect to a design variable, b , gives a sensitivity equation for a nonlinear transient heat transfer problem as,

$$\begin{aligned} & (C + K + M^+ + J_c + J_k + J_{M^+}) \cdot \frac{d\mathbf{a}_n}{db} \\ &= - \left(\frac{dC}{db} + \frac{dK}{db} + \frac{dM^+}{db} \right) \mathbf{a}_n + \frac{dM^-}{db} \mathbf{a}_{n-1} + M^- \frac{d\mathbf{a}_{n-1}}{db} + \frac{d\mathbf{q}}{db} \end{aligned} \quad (49)$$

The derivative matrices appearing in the right-hand side of Eq. 49 are new for sensitivity analysis. Generation of such matrices can be tedious and prone to mistakes. A typical derivative matrix, dC/db , is given in Appendix. Fortunately, because of the nature of approximation, those derivative matrices can be obtained in the same way as the original matrices themselves. This becomes evident by comparing Eqs. A1 and A3 in Appendix. Furthermore, it is noted that Eq. 49 is a linear equation of $\frac{d\mathbf{a}_n}{db}$, which enjoys the same left-hand side coefficient matrices as Eq. 46 . Thus, the factored matrices saved from the converged analysis, can be reused here to solve the sensitivity equation. That makes the sensitivity analysis computationally efficient.

NUMERICAL RESULTS

An academic example is used here to verify the derived equations. The space domain of the 2-D problem is a 1x1 square, which is discretized into two triangular p -version finite elements, as shown in Fig. 4. The heat source term, Q , is specifically selected so that the solution of the heat transfer problem, Eq.36, is

$$u_e(x, y, t) = xy(x-1)(y-1)t^5$$

which gives homogeneous boundary conditions and zero initial condition. Both the material properties, ρc and isotropic k , are assigned by a linear temperature relation,

$$\rho c, k = 20. + u$$

The time step is set to be 1 second and the total operational time, τ , is set to be 4 seconds.

In the numerical exercise, the orders of in-plane and the temporal polynomials are selected to be 4 and 6, respectively, for temperature interpolation, Eq. 44, whereas the orders of in-plane and the temporal polynomials are 3 and 5, respectively, for material property interpolation, Eq. 45. The total Lagrange points for the in-plane material interpolation is 10 as marked in Fig. 4. Moreover, the error is measured by the L^2 -norm¹⁵ as

$$\|e(t)\| = \left\{ \int_0^{\tau} \left[\int_{\Omega} \left[\left(\frac{\partial e}{\partial x} \right)^2 + \left(\frac{\partial e}{\partial y} \right)^2 + e^2 \right] dx dy \right] dt \right\}^{1/2}$$

where $e = u - u_e$ and u is the numerical solution.

At the end of the first time interval, $t_1 = 1$ second, the error is in the order of 10^{-4} . The error is growing with the time. At $t_2 = 2$ second, the error grows to the order of 10^{-1} . At $t_4 = 4$, the error becomes 13.31. The major source of the error is expected from deficiency in the in-plane interpolation of materials. The material property is linear in temperature. Thus, the exact order of in-plane material interpolation has to be 4 which is higher than 3, the order used in the current study. Such error will be accumulated from one time interval to the next. The results of temperature distribution are shown in Fig. 5.

Case 1

The slope of the thermal conductivity-temperature relation is considered as a design variable. Since only the matrix K depends upon this special design variable, the right-hand side of Eq.49 can be greatly reduced to a single term $-(dK / db) \mathbf{a}$. The results of the thermal sensitivity coefficients at times from 1 second to 4 seconds are shown in Fig. 6. Note that the thermal sensitivity coefficients is interpolated in the same way as the temperature; i.e.,

$$\frac{du}{db} = \chi^T(x, t) \frac{d\mathbf{a}}{db}$$

where $d\mathbf{a} / db$ is obtained from Eq. 49. Comparing with the finite differencing, the errors of the thermal sensitivity coefficients are less than 10^{-4} for all the time intervals. Note that in this example, thermal sensitivity analysis takes only 18% of the time required for one thermal analysis.

Case 2

Since in this study, the material property is a distributed function, one may then assume that the square slab is made of various materials. In this particular case, the value of k at each Lagrange point is determined by its own material table. If the slope of each material table is considered as a design variable, there are 10 independent design variables in total. They are marked in Fig. 4.

Figures 7 and 8 show the thermal sensitivity coefficients of du / db_1 and du / db_9 , where b_1 and b_9 are the slopes of the thermal conductivity-temperature relation at Lagrange points 1 and 9, respectively. The figures reveal that the design variable, b_1 , effects the change of temperature along the diagonal line, whereas the design variable, b_9 , does the area off the diagonal line more. Finally, all 10 thermal sensitivity coefficients of the temperature at the center point are collected and plotted out in Fig. 10. The picture indicates the degree of influence of individual design variable on the temperature at the center location at different time.

CONCLUSIONS

The paper uses two examples to demonstrate the derivation procedure for thermal sensitivity analysis. The continuous approach is used in the first example and the discrete approach is used in the second example. It is shown in the first example that the direct differentiation method can achieve better accuracy in thermal sensitivity analysis than the adjoint variable method. Several authors have similar observation. Furthermore, Example 1 shows that the direct results of the direct differentiation method, thermal derivatives of the temperature, are very useful in design. This particular advantage of the direct differentiation method is also demonstrated in Example 2.

The second example presented here only represented an initial attempt to find the thermal sensitivity based upon the p -version time-discontinuous Galerkin's method. Though construction of the matrix equation for thermal analysis is complicated, construction of that for thermal sensitivity analysis is rather simple. The resultant sensitivity equation is also demonstrated to be computationally efficient. However, more works are needed to develop error-control capability for thermal analysis and sensitivity analysis to ensure the quality of the p -version time-discontinuous Galerkin's method.

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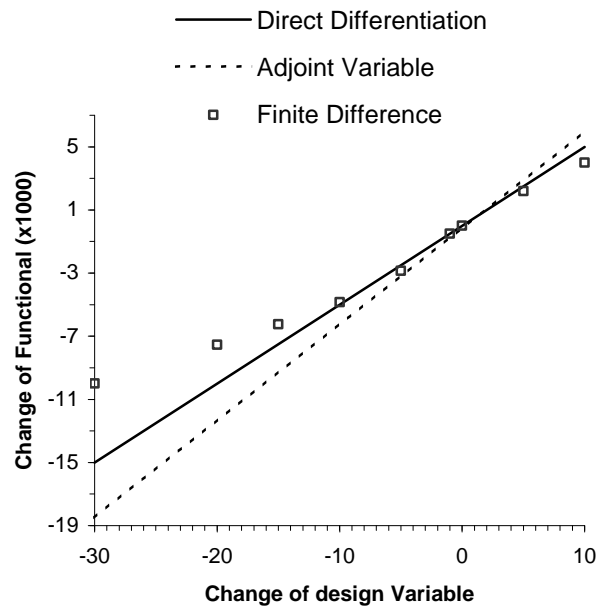


Figure 1: Thermal Design Derivatives for Press Molding with Respect to the Mold Temperature.

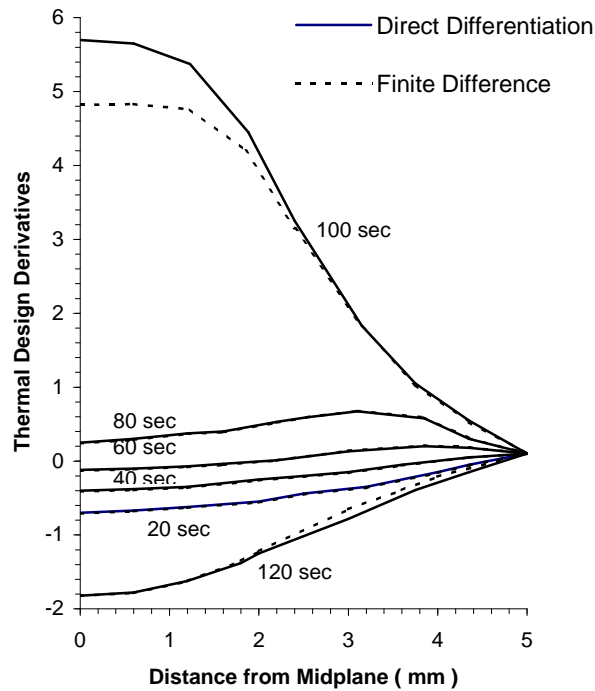


Figure 2: Profiles of Thermal Design Derivatives of Temperature with Respect to the Mold Temperature.

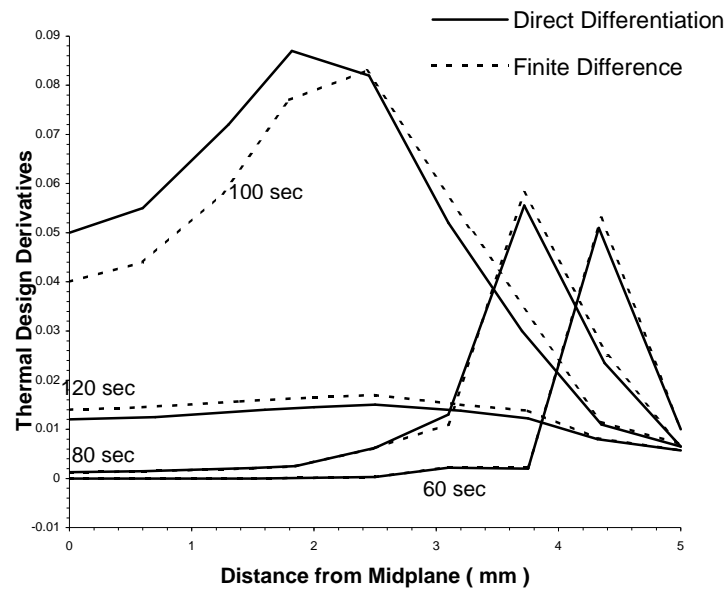


Figure 3: Profiles of Thermal Design Derivatives of the State of Cure with Respect to the Mold Temperature.

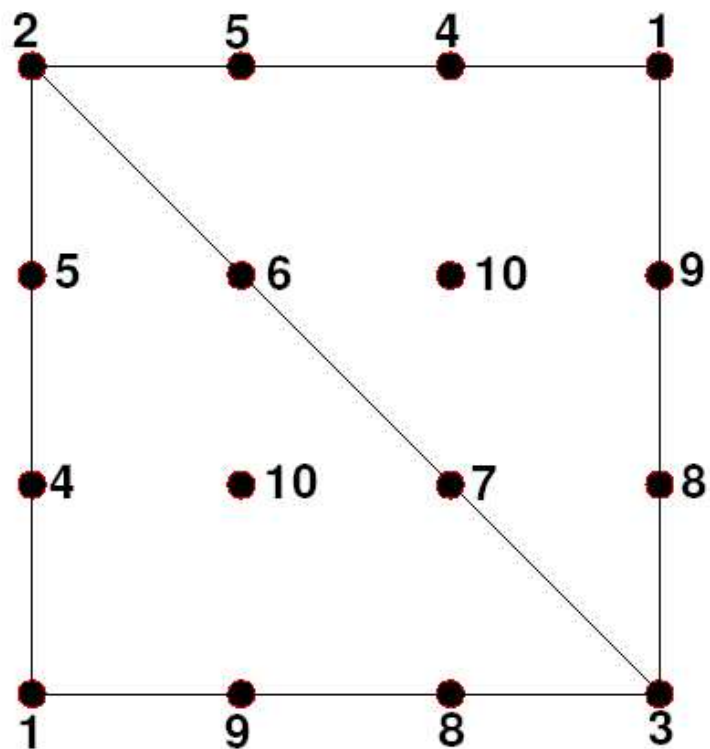


Figure 4: Meshes and Lagrange Points for Interpolation of Material Property

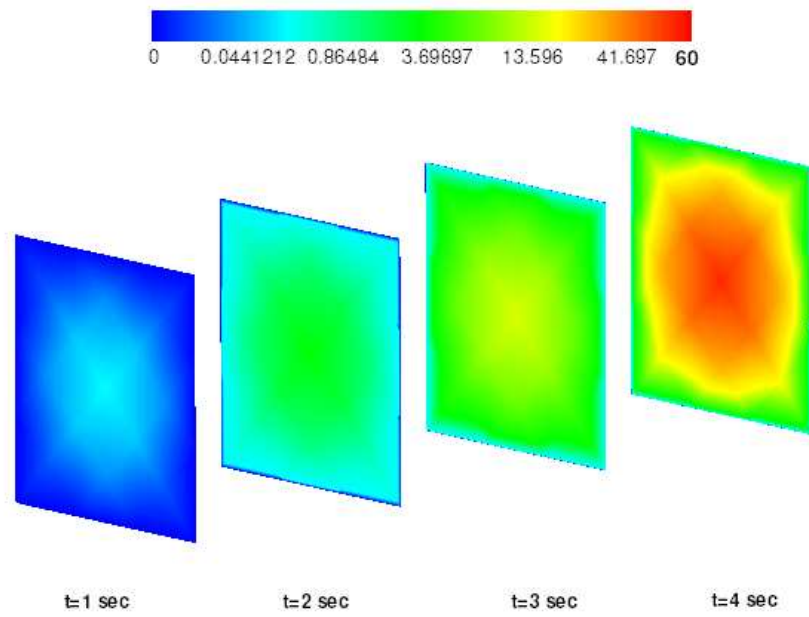


Figure 5: Temperature Distribution

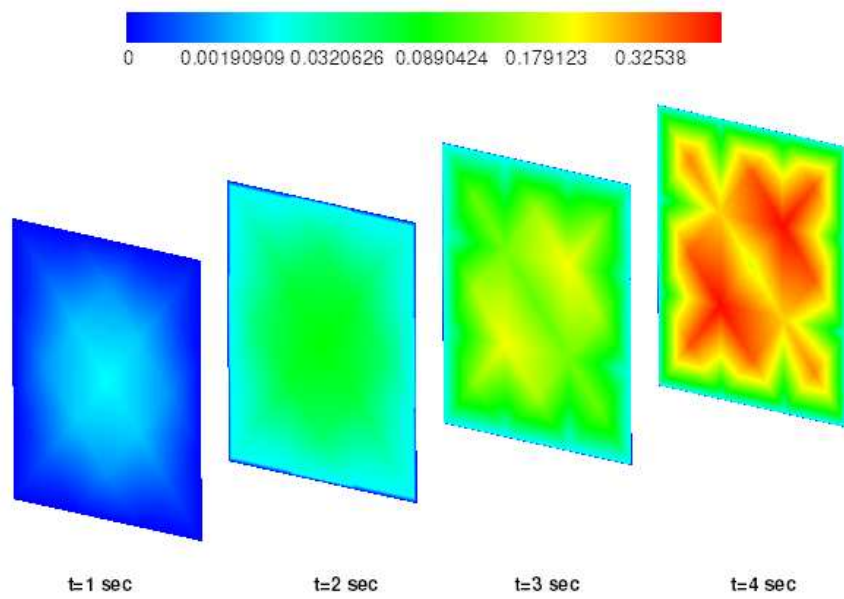


Figure 6: Coefficients of Thermal Sensitivity with Respect to Homogeneous Thermal Conductivity; $\frac{\partial u(x, y)}{\partial b}$.

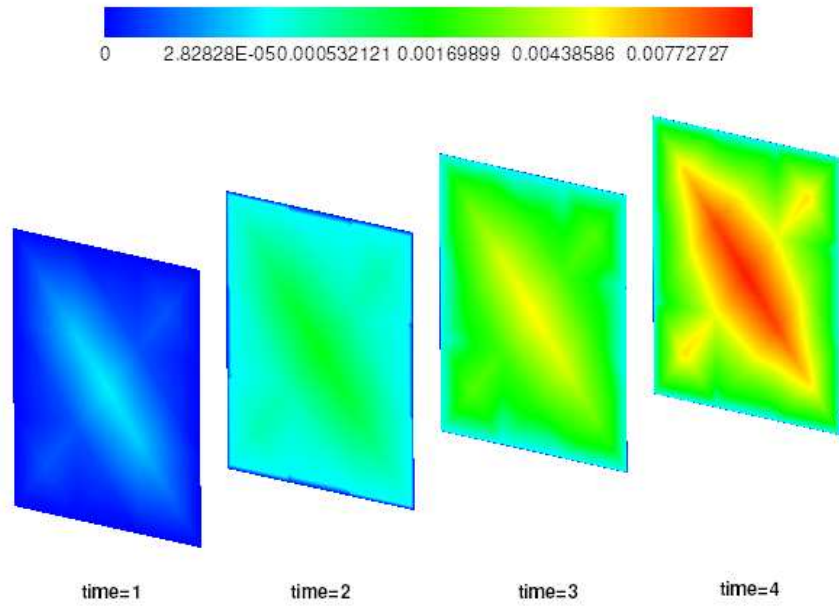


Figure 7: Coefficients of Thermal Design Sensitivity with Respect to Thermal Conductivity at Material Lagrange Point 1; $\frac{\partial u(x, y)}{\partial b_1}$.

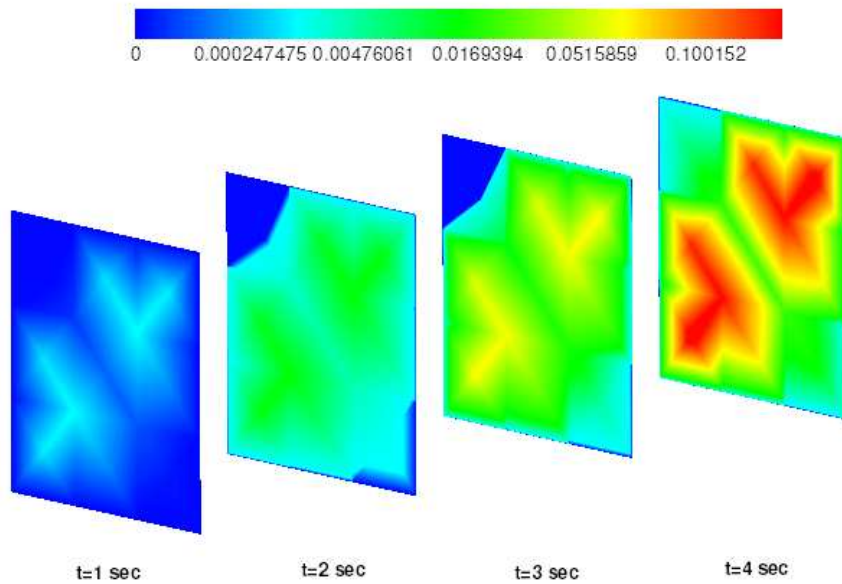


Figure 8: Coefficients of Thermal Design Sensitivity with Respect to Thermal Conductivity at Material Lagrange Point 9; $\frac{\partial u(x, y)}{\partial b_9}$.

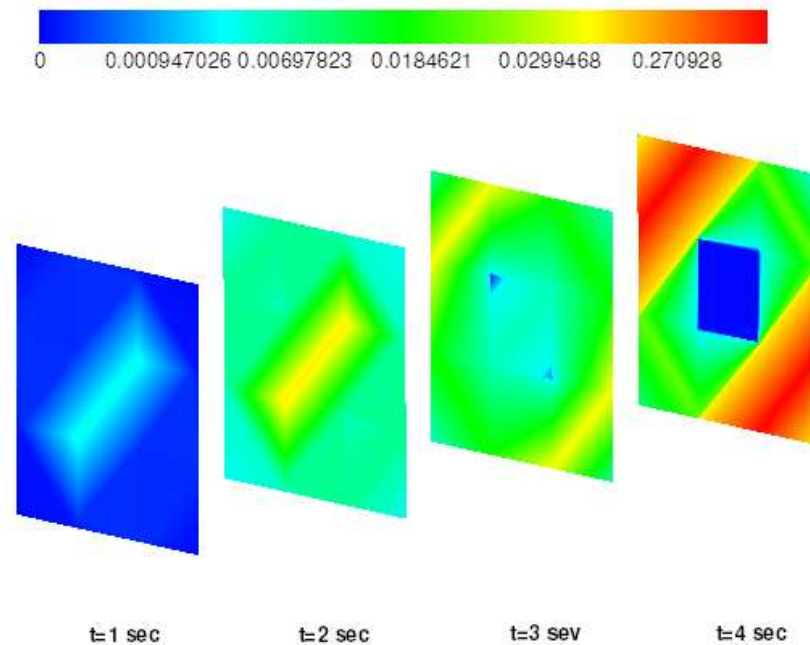


Figure 9: Coefficients of Thermal Design Sensitivity with Respect to Thermal Conductivity; $\frac{\partial u(x_c, y_c)}{\partial b_i}$; $i=1$ to 10.

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APPENDIX:

$$\begin{aligned}
C_{\Omega_e} &= \int_{t_{n-1}}^{t_n} \int_{\Omega_p} \int_{\frac{-d}{2}}^{\frac{d}{2}} \rho c \chi \frac{\partial \chi^T}{\partial t} dz dA dt \\
&= \int_{t_{n-1}}^{t_n} \int_{\Omega_e} \int_{\frac{-d}{2}}^{\frac{d}{2}} (N_c^T \delta_c) (\phi \otimes \psi \otimes \theta) \left(\phi \otimes \psi \otimes \frac{d\theta}{dt} \right)^T dz dA dt \\
&= \sum_i \sum_j \sum_k \left\{ \left(\int_{\Omega_p} \phi \phi^T N_{cpi} dA \otimes \int_{\frac{-d}{2}}^{\frac{d}{2}} \psi \psi^T N_{czk} dz \otimes \int_{t_{n-1}}^{t_n} \theta \frac{d\theta^T}{dt} N_{ctj} dt \right) \delta_{ijk} \right\}
\end{aligned} \tag{A.1}$$

$$\begin{aligned}
J_{c, \Omega_p} &= \int_{t_{n-1}}^{t_n} \int_{\Omega_p} \int_{\frac{-d}{2}}^{\frac{d}{2}} \frac{\partial(\rho p c)}{\partial a}(\chi) \frac{\partial(\chi^T \cdot a)}{\partial t} dz dA dt \\
&= \int_{t_{n-1}}^{t_n} \int_{\Omega_p} \int_{\frac{-d}{2}}^{\frac{d}{2}} N_c^T \frac{\partial \delta_c}{\partial a} (\phi \otimes \psi \otimes \theta) \left(\phi \otimes \psi \otimes \frac{d\theta}{dt} \right)^T a dz dA dt \\
&= \sum_i \sum_j \sum_k \left\{ \left[\left(\int_{\Omega_p} \phi \phi^T N_{cpi} dA \otimes \int_{\frac{-d}{2}}^{\frac{d}{2}} \psi \psi^T N_{czk} dz \otimes \int_{t_{n-1}}^{t_n} \theta \frac{d\theta^T}{dt} N_{ctj} dt \right) a \right] (\alpha_{ijk} \chi_{ijk}) \right\}
\end{aligned} \tag{A. 2}$$

$$\begin{aligned}
\frac{dC_{\Omega_p}}{db} &= \int_{t_{n-1}}^{t_n} \int_{\Omega_p} \int_{\frac{-d}{2}}^{\frac{d}{2}} \frac{\partial(\rho c)}{\partial b} \chi \frac{\partial \chi^T}{\partial t} dz dA dt \\
&= \int_{t_{n-1}}^{t_n} \int_{\Omega_e} \int_{\frac{-d}{2}}^{\frac{d}{2}} (N_c^T \frac{\partial \delta_c}{\partial b}) (\phi \otimes \psi \otimes \theta) \left(\phi \otimes \psi \otimes \frac{d\theta}{dt} \right)^T dz dA dt \\
&= \sum_i \sum_j \sum_k \left\{ \left(\int_{\Omega_p} \phi \phi^T N_{cpi} dA \otimes \int_{\frac{-d}{2}}^{\frac{d}{2}} \psi \psi^T N_{czk} dz \otimes \int_{t_{n-1}}^{t_n} \theta \frac{d\theta^T}{dt} N_{ctj} dt \right) \frac{\partial \delta_{ijk}}{\partial b} \right\}
\end{aligned} \tag{A.3}$$